

On the complicate structure of a condensate for the Bose fluid in a vessel

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We show that the ground state of the Bose fluid in a vessel-parallelepiped can be characterized not only by the quantum numbers $\mathbf{p} = (\pm 2\pi l_x/L_x, \pm 2\pi l_y/L_y, \pm 2\pi l_z/L_z)$ ($l_x, l_y, l_z = 1, 2, 3, \dots$) of an expansion in the eigenfunctions $e^{i\mathbf{p}\mathbf{r}}$ of a free particle, but also by the quantum numbers $\mathbf{k}_l = (\pi l_x/L_x, \pi l_y/L_y, \pi l_z/L_z)$ of an expansion in the eigenfunctions $\sin(k_{l_x}x)\sin(k_{l_y}y)\sin(k_{l_z}z)$ of a particle in the box. In the latter case, the one-particle condensate “is dispersed” over many lower levels with odd l_x, l_y, l_z . 53% atoms of the condensate occupy the lowest level with $\mathbf{k} = (\pi/L_x, \pi/L_y, \pi/L_z)$. The sum of condensates on all levels is determined by the same formula $N_c/N = \rho_\infty$, as that for the condensate on the level with $p = 0$. The proposed \mathbf{k} -representation supplements the traditional one (with the condensate on the level $\epsilon = (\hbar p)^2/2m = 0$) and allows one to consider the microstructure of a system from another side.

Keywords Composite condensate, Bose fluid, Zero boundary conditions

1 Introduction

The problem of a condensate in the Bose fluid attracts attention as before. The condensate was predicted theoretically [1]–[3] and was then discovered experimentally. Moreover, the experimental values [4, 5] agree sufficiently well with theoretical ones [3, 6]–[11]. Intensively are studied the condensates in rarefied gases in traps. But some difficulties exist also. In particular, all the calculations of the condensate possess shortcomings decreasing the accuracy of results: sometimes, a lot of fitting parameters are used [8], or the correlation corrections are large [7, 10]; in the most exact Monte Carlo simulations [6, 9, 11], the interatomic potential is applied, though it is only effective at small distances and is known approximately.

In addition, we meet the difficulty, which remains usually unnoticeable. A condensate in the Bose fluid is considered as the “macroscopic number of atoms with zero momentum.” However, the fluid is placed always in a vessel, and the uncertainty relation $\hbar\Delta p_x\Delta x \geq \hbar/2$ implies that the momentum of an atom cannot be zero due to the uncertainty $\Delta p_x \geq 1/2L$. This point is obviously clear: the momentum is defined for translation-invariant systems, whereas the walls break the translational invariance, and the momentum of an atom is not conserved due to the collisions with walls. In addition, the momentum takes the discrete values $\mathbf{p} = 2\pi(j_x/L_x, j_y/L_y, j_z/L_z)$ in the standard approach, and its uncertainty $\geq 1/2L$ is comparable with the distance between adjacent values. Therefore, the collection of discrete levels is transformed in a collection of bands or even in a single band. This means that the momentum is a “bad” quantum number. However, this circumstance creates no significant problem, because we can consider \mathbf{p} as an eigenvalue of the Hamiltonian ($\epsilon = (\hbar p)^2/2m$) and

can use the traditional formalism. But it is possible to go along a nontraditional way with the construction of another approach to the description of the microstructure of systems. Such new approach will be considered in what follows.

2 Structure of a condensate for the Bose fluid in a vessel

Consider the Bose fluid in a vessel at $T = 0$. In the standard approach with periodic boundary conditions (BCs), the condensate $n_0 = N_{\mathbf{p}=0}/N$ is determined from the formula

$$\frac{N_{\mathbf{p}}}{N} = \int d\mathbf{r}_1 d\mathbf{r}_2 \rho(\mathbf{r}_1, \mathbf{r}_2) \frac{e^{-i\mathbf{p}(\mathbf{r}_1 - \mathbf{r}_2)}}{V^2}, \quad (1)$$

where N is the total number of identical Bose particles, V is the volume of the system, $\rho(\mathbf{r}_1, \mathbf{r}_2)$ is the one-particle density matrix,

$$\rho(\mathbf{r}_a, \mathbf{r}_b) = V \int d\mathbf{r}_2 \dots d\mathbf{r}_N \Psi_0^*(\mathbf{r}_a, \mathbf{r}_2, \dots, \mathbf{r}_N) \Psi_0(\mathbf{r}_b, \mathbf{r}_2, \dots, \mathbf{r}_N), \quad (2)$$

and Ψ_0 is the wave function of the ground state of the system. For an infinite system, we have $\rho(\mathbf{r}_1, \mathbf{r}_2) = \rho(|\mathbf{r}_1 - \mathbf{r}_2|)$ due to the translational invariance and the isotropy. Therefore,

$$n_0 = \frac{N_{\mathbf{p}=0}}{N} = \frac{1}{V^2} \int d\mathbf{r}_1 d\mathbf{r}_2 \rho(|\mathbf{r}_1 - \mathbf{r}_2|) = \rho(|\mathbf{r}_1 - \mathbf{r}_2| \rightarrow \infty) \equiv \rho_\infty. \quad (3)$$

The presented definition of the condensate follows from the expansion

$$\Psi(\mathbf{r}) = \int d\mathbf{p} a(\mathbf{p}) e^{i\mathbf{p}\mathbf{r}} (2\pi)^{-3} \quad (4)$$

in the eigenfunctions $e^{i\mathbf{p}\mathbf{r}}$ of the momentum operator, which form the complete collection of orthonormalized basis functions of the continuous spectrum. The exponential function $e^{i\mathbf{p}\mathbf{r}}$ is an eigenfunction of the Hamiltonian and the momentum operator for a free particle in the infinite or finite closed volume. The closed ring systems are described by periodic BCs and are realized in the nature only in the one- or two-dimensional case.

Consider the finite-size systems with nonperiodic BCs. In particular, the boundary conditions for the three-dimensional systems are always nonperiodic. As was noted in [12], the expansion for the system in a box should be performed in an eigenfunctions of this system. Work [12] gives the solution for N point Bose particles in a box-cube $L \times L \times L$ characterized by an interatomic potential in the form of the δ -function. The BCs were taken to be $\mathbf{n}\nabla\psi = 0$. It was found that all atoms are on the lowest level at a repulsive potential. At an attractive potential, the atoms are distributed over ($\sim N^{2/5}$) lower levels, but with the microscopic ($\sim N^{3/5}$) population of each level. In this case, the condensate exists in the “generalized” sense [12]: the total number of atoms on those levels turns out macroscopic.

But the real atoms are not point-like and possess a smoother potential, than the δ -function. Therefore, the wave functions may have a different structure as compared with that of the solutions in [12]. We may expect also a different solution for the condensate. We now consider such realistic system of Bose particles in the box $L_x \times L_y \times L_z$. For simplicity, let us consider firstly the 1D case. We model the potential of a wall as a step with finite height:

$$U_w(x) = \begin{cases} U > 0 & x \leq 0, x \geq L \\ 0 & 0 < x < L. \end{cases} \quad (5)$$

Let the potentials of both walls be identical (their distinction will not lead to basic changes). The eigenfunctions of a free particle in such a box are known [14]:

$$\Psi_l(x) = \begin{cases} c_l \sin(\delta_l) e^{\kappa_l x}, & x \leq 0 \\ c_l \sin(k_l x + \delta_l), & 0 < x < L_x \\ c_l (-1)^{l+1} \sin(\delta_l) e^{-\kappa_l (x-L)}, & x \geq L_x, \end{cases} \quad (6)$$

$$k_l = \sqrt{2mE_l}/\hbar = \pi l/L_x - 2\delta_l/L_x, \quad (7)$$

$$\kappa_l = \sqrt{2m(U - E_l)}/\hbar > 0, \quad \delta_l = \arcsin(\gamma_x k_l L_x/2), \quad (8)$$

$$c_l = \left(\frac{(\sin \delta_l)^2}{\kappa_l} + \frac{L_x}{2} + \frac{\sin(2\delta_l)}{2k_l} \right)^{-1/2} \approx \sqrt{\frac{2}{L_x}}. \quad (9)$$

Here, $l = 1, 2, 3, \dots$, $\gamma_x = \frac{\hbar}{L_x} \sqrt{\frac{2}{mU}}$, and the values of \arcsin are taken between 0 and $\pi/2$. The boundary conditions involve the continuity of $\Psi_l(x)$, $\Psi'_l(x)$ and are more physical than the BCs $\mathbf{n}\nabla\psi = 0$ in [12]. For great systems, $\gamma_x \ll 1$: for He^4 atoms at $U = 100$ K and $L_x = 10$ cm, we have $\gamma_x \approx 4.9 \times 10^{-10}$. For $l \ll 1/\pi\gamma_x$, we obtain

$$k_l \approx lk_1 = l(1 - \gamma_x)\pi/L_x, \quad \delta_l \approx l\delta_1 = l\pi\gamma_x/2. \quad (10)$$

Solutions (6) describe bound states with discrete spectrum. Here, we omit the solutions $\Psi_f(x)$ with continuous spectrum, which correspond to the infinite motion with $E > U$. The solutions for the continuous and discrete spectra are eigenfunctions of the Hermitian operator (Hamiltonian). By the theorems of quantum mechanics, these functions form the complete orthonormalized collection of basis functions, in which any function $\Psi(x)$ with the appropriate smooth properties and given on the interval $x \in]-\infty, \infty[$ can be expanded. Therefore, any solution for a free particle localized in a 1D box (5) can be written in the form

$$\Psi(x) = \sum_l b_l \Psi_l(x), \quad b_l = \int_{-\infty}^{\infty} dx \Psi(x) \Psi_l^*(x), \quad (11)$$

and the probability for the particle in the state $\Psi(x)$ to have the wave number k_l is equal to $|b_l|^2$.

Let us consider the Bose fluid in a vessel. In the presence of a vessel, the momentum is not a quite good quantum number. Therefore, we are not based on the momentum operator, while choosing the eigenvalues for the expansion of the density matrix. Then the exponents $e^{ip_x x}$ lose the status of exceptional functions: now, we can use only the eigenfunctions of the Hamiltonian of a free particle, which are the collections of all possible linear combinations of the form $ae^{ip_x x} + be^{-ip_x x}$ with different p_x , where p_x are multiple to $2\pi/L$. Among those collections, we separate two ones: first, the exponential functions $e^{ip_x x}$ (because they give solutions for the quasiparticles in the form of traveling waves, and the phonons in real systems are namely traveling wave packets, rather than standing waves; we call it **p**-representation), and, second, the sines $\sin(k_l x + \delta_l)$ (6) (since they take the boundary conditions into account, by ensuring the decrease of the wave functions near the boundary; we call it the **k**-representation). Here, the wave vectors **k** and **p** are similar to the momentum, but they are not the momentum, but a quantum numbers of the Hamiltonian. None of these collections of eigenfunctions can be called definitely the best. In our view, the exponential functions describe better the quasiparticles, whereas the sines do the ground state and the condensate.

In the \mathbf{p} -representation, we obtain obviously the well-known results with the condensate on a level with $\mathbf{p} = 0$. Of a significant interest is the \mathbf{k} -representation based on the functions $\Psi_l(x)$ (6). We now consider it in more details. The wave vector takes the values

$$\mathbf{k} = \mathbf{k}_1 = \left(\frac{\pi l_x - 2\delta_{l_x}}{L_x}, \frac{\pi l_y - 2\delta_{l_y}}{L_y}, \frac{\pi l_z - 2\delta_{l_z}}{L_z} \right) \quad (12)$$

with $l_x, l_y, l_z = 1, 2, 3, \dots$. We omit the negative components, since the wave function of a particle for them differs only by a sign (these are equivalent states). For the Bose fluid states of the discrete spectrum, the number of particles with the wave vector \mathbf{k} is

$$\frac{N_{\mathbf{k}}}{N} = \frac{1}{V} \int_{-\infty}^{\infty} d\mathbf{r}_1 d\mathbf{r}_2 \rho(\mathbf{r}_1, \mathbf{r}_2) \Psi_{l_x}^*(x_1) \Psi_{l_x}(x_2) \Psi_{l_y}^*(y_1) \Psi_{l_y}(y_2) \Psi_{l_z}^*(z_1) \Psi_{l_z}(z_2). \quad (13)$$

Let us verify the correctness of the coefficient V^{-1} . The property of eigenfunctions

$$\sum_1 \Psi_1^*(\mathbf{r}_1) \Psi_1(\mathbf{r}_2) + \int d\mathbf{f} \Psi_{\mathbf{f}}^*(\mathbf{r}_1) \Psi_{\mathbf{f}}(\mathbf{r}_2) = \delta(\mathbf{r}_1 - \mathbf{r}_2) \quad (14)$$

and the normalization of Ψ_0 yield

$$\sum_{\mathbf{k}} \frac{N_{\mathbf{k}}}{N} + \int d\mathbf{f} \frac{N_{\mathbf{f}}}{N} = 1, \quad (15)$$

i.e., the coefficient is proper. The integral over the continuous spectrum is probably much less than 1.

Let us determine $N_{\mathbf{k}}$. According to (13), we need to integrate over the whole volume, inside and outside of the box. But we do not know the solution for Ψ_0 outside of the box. However, it is clear that this solution decreases exponentially, with the penetration distance $\sim 1 \text{ \AA}$ for realistic walls. Therefore, we neglect the region outside of the box. Then, in the 3D case, we obtain

$$\begin{aligned} \frac{N_{\mathbf{k}_1}}{N} &= \frac{1}{V} \int_0^{L_x, L_y, L_z} d\mathbf{r}_1 d\mathbf{r}_2 \rho(\mathbf{r}_1, \mathbf{r}_2) c_{l_x}^2 c_{l_y}^2 c_{l_z}^2 \sin(k_{l_x} x_1 + \delta_{l_x}) \sin(k_{l_x} x_2 + \delta_{l_x}) \\ &\times \sin(k_{l_y} y_1 + \delta_{l_y}) \sin(k_{l_y} y_2 + \delta_{l_y}) \sin(k_{l_z} z_1 + \delta_{l_z}) \sin(k_{l_z} z_2 + \delta_{l_z}). \end{aligned} \quad (16)$$

We now have $\rho(\mathbf{r}_1, \mathbf{r}_2) \neq \rho(\mathbf{r}_1 - \mathbf{r}_2)$, generally speaking. At distances from the wall much larger than the interatomic distance R , the properties of Ψ_0 are the same [13] as those for an infinite system. Therefore, at \mathbf{r}_1 and \mathbf{r}_2 far from the walls and $|\mathbf{r}_1 - \mathbf{r}_2| \gg R$, the relation $\rho(\mathbf{r}_1, \mathbf{r}_2) = \rho_{\infty} = \text{const}$ is true. With regard for it, relation (16) yields

$$\frac{N_{\mathbf{k}_1}}{N} = \left(\frac{8c_{l_x} c_{l_y} c_{l_z} \cos \delta_{l_x} \cos \delta_{l_y} \cos \delta_{l_z}}{k_{l_x} k_{l_y} k_{l_z}} \right)^2 \frac{\rho_{\infty}}{V}, \quad (17)$$

if l_x, l_y, l_z are odd, and $N_{\mathbf{k}_1}/N = 0$, if at least one of l_x, l_y, l_z is even. Let us consider odd l_x, l_y, l_z . The value of $N_{\mathbf{k}_1}$ is large at small \mathbf{k}_1 , when relations (10) hold. In this case,

$$\frac{N_{\mathbf{k}_1}}{N} \approx \frac{8^3 \rho_{\infty}}{\pi^6 l_x^2 l_y^2 l_z^2}. \quad (18)$$

Since $\rho_{\infty} \sim 1$, we obtain the condensate $N_{\mathbf{k}_1} \sim N$ for all levels with small l_x, l_y, l_z . The sum of condensates on all levels

$$n_c = \sum_{\mathbf{k}} \frac{N_{\mathbf{k}}}{N} \approx \frac{8^3 \rho_{\infty}}{\pi^6} \sum_{j_x, j_y, j_z} \frac{1}{(1 + 2j_x)^2 (1 + 2j_y)^2 (1 + 2j_z)^2} = \rho_{\infty} \quad (19)$$

$(j_x, j_y, j_z = 0, 1, 2, 3, \dots)$ is exactly equal to the condensate on the level $\mathbf{p} = 0$ for the \mathbf{p} -representation. This interesting property is general. We denote $V^{-1/2} = |\mathbf{r}\rangle$, $\rho_\infty = \hat{\rho}$, $\Psi_{l_x}(x)\Psi_{l_y}(y)\Psi_{l_z}(z) = |\mathbf{l}\rangle$ and expand the function $\Psi(\mathbf{r})$, equal to $V^{-1/2}$ in the box and to zero outside of it, in the functions $|\mathbf{l}\rangle$ and the continuous-spectrum functions of a particle in the box. The latter enter the expansion with zero coefficients. Therefore, $\Psi(\mathbf{r}) = \sum_{\mathbf{l}} c_{\mathbf{l}} |\mathbf{l}\rangle$, $c_{\mathbf{l}} = \langle \mathbf{r} | \mathbf{l} \rangle$. Then, in the approximation $\rho(\mathbf{r}_1, \mathbf{r}_2) = \rho_\infty$, we have

$$\begin{aligned} \sum_{\mathbf{p}} N_{\mathbf{p}}/N &= N_{\mathbf{p}=0}/N = \rho_\infty = \int d\mathbf{r} \rho_\infty (e^{i\mathbf{p}\mathbf{r}}/V)|_{\mathbf{p} \rightarrow 0} \\ &= \langle \mathbf{r} | \hat{\rho} | \mathbf{r} \rangle = \langle \mathbf{r} | \mathbf{l} \rangle \langle \mathbf{l} | \hat{\rho} | \mathbf{m} \rangle \langle \mathbf{m} | \mathbf{r} \rangle = \sum_{\mathbf{l}, \mathbf{m}} c_{\mathbf{l}} c_{\mathbf{m}}^* \langle \mathbf{l} | \hat{\rho} | \mathbf{m} \rangle \\ &= \sum_{\mathbf{l}} |c_{\mathbf{l}}|^2 \langle \mathbf{l} | \hat{\rho} | \mathbf{l} \rangle = \rho_\infty \sum_{\mathbf{l}} |c_{\mathbf{l}}|^2 = \sum_{\mathbf{k}_1} N_{\mathbf{k}_1}/N. \end{aligned} \quad (20)$$

We do not use the specific form of the functions $|\mathbf{l}\rangle$. Therefore, the summary condensate $\sum_{\mathbf{k}_1} N_{\mathbf{k}_1}/N$ is the same for any basis of eigenfunctions. This property is related to the fact that the constant ρ_∞ can be expanded in various bases.

The real value of n_c is somewhat less than that in (19). The condensate corresponds to the macroscopic filling of a level, but sum (19) includes also large values of j_x, j_y, j_z , at which the filling is small. We call the level macroscopically filled, if $N_{\mathbf{k}} > q_c N$. The value of q_c is conditional, but the estimate $q_c \sim (1-100) \times N^{-1/3}$ seems reasonable. The numerical analysis indicates that, at $q_c = 0.001$, we have $n_c \approx 0.914\rho_\infty$ and the number of condensate levels $N_c = 49$. At $q_c = 10^{-6}$, we obtain $n_c \approx 0.994\rho_\infty$ and $N_c = 3920$. Whereas $n_c \approx 0.999\rho_\infty$ and $N_c \approx 61400$ at $q_c = 10^{-8}$. For great systems $N^{1/3} \gtrsim 10^8$. In this case $q_c \sim 10^{-6}-10^{-8}$, and n_c differs slightly from $n_c = \rho_\infty$ (19).

It is clear that, for the 1D and 2D cases, the properties of the condensate are analogous.

For a different shape of the vessel, we need to use different basis functions at the expansion, but the summary condensate is not changed, according to (20). If we consider the realistic potential of a wall (smoother than that of a step and like the interaction potential of two helium atoms), the summary condensate is not changed as well, but, probably, will be more strongly dispersed over levels.

The additional information is given by the exact wave function Ψ_0 [13] of a system of N interacting Bose particles in a box-parallelepiped with impermeable walls ($U = \infty$):

$$\Psi_0 = \Psi_0^\infty e^{S_w^{(1)}} \prod_j \{ \sin(k_{1x} x_j) \sin(k_{1y} y_j) \sin(k_{1z} z_j) \}, \quad (21)$$

$$S_w^{(1)} = \sum_{\mathbf{q} \neq 0} S_1^{(1)}(\mathbf{q}) \rho_{-\mathbf{q}} + \sum_{\mathbf{q}, \mathbf{q}_1 \neq 0}^{\mathbf{q} + \mathbf{q}_1 \neq 0} \frac{S_2^{(1)}(\mathbf{q}, \mathbf{q}_1)}{\sqrt{N}} \rho_{\mathbf{q}_1} \rho_{-\mathbf{q}_1 - \mathbf{q}} + \dots, \quad (22)$$

where $\mathbf{k}_1 = (k_{1x}, k_{1y}, k_{1z}) = (\pi/L_x, \pi/L_y, \pi/L_z)$, $\rho_{\mathbf{k}} = \frac{1}{\sqrt{N}} \sum_{j=1}^N e^{-i\mathbf{k}\mathbf{r}_j}$, and Ψ_0^∞ is the well-known solution [15] for Ψ_0 in the thermodynamic limit:

$$\ln \Psi_0^\infty = \sum_{\mathbf{q}_1 \neq 0} \frac{a_2(\mathbf{q}_1)}{2!} \rho_{\mathbf{q}_1} \rho_{-\mathbf{q}_1} + \sum_{\mathbf{q}_1, \mathbf{q}_2 \neq 0}^{\mathbf{q}_1 + \mathbf{q}_2 \neq 0} \frac{a_3(\mathbf{q}_1, \mathbf{q}_2)}{3! \sqrt{N}} \rho_{\mathbf{q}_1} \rho_{\mathbf{q}_2} \rho_{-\mathbf{q}_1 - \mathbf{q}_2} + \dots \quad (23)$$

The components of \mathbf{q} and \mathbf{q}_j are multiple to $2\pi/L$. If we expand both exponential functions in (21) in a series, represent $\rho_{\mathbf{k}}$ in terms of cosines and sines, and convolve them with sines

from the bare product of sines in (21), we obtain the sum of products of N sines and cosines with wave vectors multiple to π/L . This yields two conclusions for particles in a box. 1) The wave vectors of interacting particles “are quantized” in the same way like those of free particles. 2) If the interatomic interaction is switched-off, Ψ_0 is reduced to a product of sines, i.e., to the solution for the ground state of N free particles, when all particles are in the condensate with $\mathbf{k} = \mathbf{k}_1$. The structure of condensate (19) agrees with this solution: if the interaction tends to zero, the atoms from above-condensate levels “fall” on the condensate levels; if the interaction is switched-off completely, the condensate levels become empty by jump: the atoms transit to the lowest level with $\mathbf{k} = \mathbf{k}_1$. But if the condensate is defined in the standard way (1), we cannot obtain N particles on the level with $\mathbf{k} = \mathbf{k}_1$ at the switching-off of the interaction. In this relation, the standard definition of a condensate is worse. The condensate measured in experiment is, in fact, the quantity ρ_∞ .

Notice that the composite condensate (19) belongs to the generalized condensates, which was considered in several works, but only for free particles or point-like potentials or cyclic BCs (see, f.e., the recent paper [16]).

Let us compare the formulas for the number of above-condensate atoms, $N_{\mathbf{p}}$, in the \mathbf{k} - and \mathbf{p} -representations for $k, p \gg \pi/L$. Let us expand the density matrix in a Fourier series:

$$\rho(\mathbf{r}_1 - \mathbf{r}_2) = \frac{1}{V^*} \sum_{\mathbf{q}} f(\mathbf{q}) e^{i\mathbf{q}(\mathbf{r}_1 - \mathbf{r}_2)}. \quad (24)$$

For the \mathbf{p} -representation, we use periodic BCs. Then $V^* = V$, and \mathbf{q} runs the values $2\pi(j_x/L_x, j_y/L_y, j_z/L_z)$. Relation (1) yields

$$N_{\mathbf{p}} = f(\mathbf{p})N/V. \quad (25)$$

For the \mathbf{k} -representation, $V^* = 8V$, and \mathbf{q} runs the values $\pi(j_x/L_x, j_y/L_y, j_z/L_z)$, and relations (16) and (24) yield

$$N_{\mathbf{k}} = r_1 f(\mathbf{k})N/V, \quad r_1 = r_{l_x} r_{l_y} r_{l_z}, \quad (26)$$

$$r_{l_x} = \frac{1}{6} + \frac{\cos^2 \delta_{l_x}}{3} + \frac{\sin^2 \delta_{l_x}}{2\delta_{l_x}^2}, \quad (27)$$

$l_x = 1, 2, \dots, l_x^{max} - 1$. The value of $l_x^{max} = 1/\delta_1$ can be determined from the condition $\delta_{l_x^{max}} = \pi/2$ and gives the maximum value of k_{l_x} . The analogous result holds for the y - and z -components. The vectors $\mathbf{k} > \mathbf{k}^{max}$ correspond to the continuous spectrum. At $\mathbf{k} \leq \mathbf{k}^{max}/2$ (for all components), $r_1 \approx 1$ is true. At larger \mathbf{k} , r_1 decreases, as \mathbf{k} increases, and $r_1(\mathbf{k}^{max}) \approx 0.05$. For He^4 atoms at $U = 25$ K, we have $k^{max} = \sqrt{6mU}/\hbar \approx 7.2 \text{ \AA}^{-1}$, which equals to the threshold momentum $k^m \approx 3.6 \text{ \AA}^{-1}$ of the dispersion curve. We do not exclude that this property explain the threshold. Thus, $r_1 \approx 1$ for all \mathbf{k} for which $f(\mathbf{k})$ is not too small, and the formulas for $N_{\mathbf{k}}$ and $N_{\mathbf{p}}$ are identical. In view of the positiveness of the components of \mathbf{k} , we have $\sum_{\mathbf{k}} = \sum_{\mathbf{p}}$ for narrow bands Δk and Δp at $p = k$. Therefore, for $\mathbf{k}, \mathbf{p} \leq \mathbf{k}^{max}/2$, the numbers of above-condensate atoms in the \mathbf{k} - and \mathbf{p} -representations are the same ($\sum_{\mathbf{k}} N_{\mathbf{k}} \approx f(\mathbf{k})Nk^2\Delta k/(2\pi^2)$).

According to [13], the solution for the wave function Ψ_0 under the zero BCs differs from that under the cyclic BCs. In view of this, the values of ρ_∞ must also be different. Hence, the amount of the condensate and the number of above-condensate atoms under the zero BCs must differ from those under the cyclic BCs, though the formulas are identical. However, we have not calculated ρ_∞ in the present work.

3 Conclusion

The analysis shows that the presence of boundaries allow one to propose the new definition of the condensate. At this definition, the condensate is dispersed over many lowest atomic levels. This effect is related to that the walls of a vessel play the role of a resonator and affect the spectrum of eigenmodes of the system.

The proposed \mathbf{k} -representation is equivalent, on the whole, to the traditional ones, but it allows one to observe new properties of a system, which are hidden, if the ordinary \mathbf{p} -representation is used.

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- [1] A. Einstein, Sitzungsber. preuss. Akad. Wiss. **1**, 3 (1925).
- [2] N.N. Bogoliubov, J. Phys. USSR **11**, 23 (1947).
- [3] L. Penrose and O. Onsager, Phys. Rev. **104**, 576 (1956).
- [4] I.V. Bogoyavlensky, L.V. Karnatsevich, G.A. Kozlov, and A.V. Puchkov, Fiz. Niz. Temp. **16**, 139 (1990).
- [5] H.R. Glyde, R.T. Azuah, and W.G. Stirling, Phys. Rev. B **62**, 14337 (2000).
- [6] M.H. Kalos, M.A. Lee, P.A. Whitlock, and G.V. Chester, Phys. Rev. B **24**, 115 (1981).
- [7] I.A. Vakarchuk, Theor. Math. Phys. **82**, 308 (1990).
- [8] L. Reatto, G.L. Masserini, and S.A. Vitiello, Physica B **197**, 189 (1994).
- [9] D.M. Ceperley, Rev. Mod. Phys. **67**, 279 (1995).
- [10] M. Tomchenko, Low Temp. Phys. **32**, 38 (2006).
- [11] R. Rota, J. Boronat, J. Low Temp. Phys. **166**, 21 (2012).
- [12] M.D. Girardeau, J. Math. Phys. **6**, 1083 (1965).
- [13] M.D. Tomchenko, submitted in Phys. Rev. B, arXiv:cond-mat/1201.1845.
- [14] L.D. Landau, E.M. Lifshitz, *Quantum Mechanics. Non-Relativistic Theory* (Pergamon, New York, 1980).
- [15] I.A. Vakarchuk and I.R. Yukhnovskii, Theor. Math. Phys. **40**, 626 (1979).
- [16] W.J. Mullin, A.R. Sakhel, J. Low Temp. Phys. **166**, 125 (2012).